IV International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2015
E. Oñate, M. Bischoff, D.R.J. Owen, P. Wriggers & T. Zohdi (Eds)

COUPLING OF PARTICLE-BASED AND GRID-BASED METHODS WITHIN OBJECT-ORIENTED MULTI-PHYSICS CFD FRAMEWORK

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Key words: Molecular Dynamics, Hypersonic Flows, Boltzmann-Kinetic Models

Abstract. A novel multi-physics approach involving mesh-based methods for kinetic-Boltzmann equations coupled with molecular dynamics (MD) simulations of thermal relaxation is introduced. The particle method, its parallel performance and the implementation in MΦC are discussed, including the unification and re-use of the source code for different methods and models. The hypersonic partially rarefied flow of a diatomic gas around a sphere and a spaceplane configuration are considered as examples, providing details about the thermal non-equilibrium conditions to be modelled using MD simulations. The MD results show that existing empirical models may not provide sufficient accuracy for the gas flow in strong expansions and that the proposed method provides a mechanism for improving the accuracy.

1 INTRODUCTION

The multi-physics solver MΦC[1, 2, 3], developed within the CFD Laboratory at the University of Liverpool was designed for hybrid simulations with a coupling of numerical methods for different mathematical models in different parts of the flow domain. A key feature of the framework is the object-oriented design, i.e. the framework constitutes a library of C++ classes on top of which a range of particle-based methods (Molecular-Dynamics, Vortex Particle method) as well as mesh-based methods for the Navier-Stokes

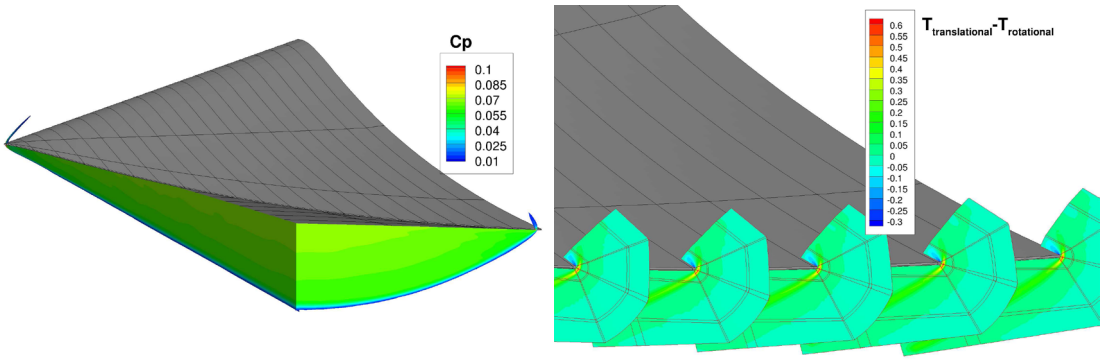


Figure 1: Hybrid kinetic-Boltzmann/Navier-Stokes simulation of Mach 8 flow around waverider

equations and the kinetic Boltzmann equations (Shakhov/Rykov-BGK[4, 5] and Ellipsoidal Statistical (ES) models[6]) were built. The design enables a large degree of re-use of source code for different methods as well as prototyping of novel coupling approaches. In previous works, the framework was demonstrated for coupled Navier-Stokes/Molecular Dynamics problems involving nano-scale flow of liquids[1, 2] as well as coupled Navier-Stokes/kinetic-Boltzmann simulations[3].

The Navier-Stokes equations form the baseline level mathematical model for the vast majority of Computational Fluid Dynamics (CFD) simulations, since the assumptions upon which the equations are based are satisfied in continuum-flow cases with weak thermodynamic non-equilibrium. MΦC was developed for the simulation of complex flows with a multi-scale character and strong thermodynamic non-equilibrium, including rarefaction effects. An important application is the modelling of high-speed, hypersonic flows around aerospace vehicles such as shown in Figure 1. The flow at Mach 8 around a waverider hypersonic cruise vehicle develops a strong shock wave on the underside of the vehicle with high-pressure air captured in a region bounded by the vehicle surface and the shock wave. Around the blunt leading-edges of the vehicle, the air previously compressed and heated by the bow shock wave leaks away towards the upper surface, creating a local area of strong expansion. Accurate modelling of these effects requires more detailed models than Navier-Stokes. On the right-hand side of Figure 1, the flow in the vicinity of the vehicle leading edge was modelled using a kinetic Boltzmann model (diatomic ES model). In the shock wave as well as the strong expansion regions, strong thermodynamic effects occur with the rotational temperature of the diatomic molecules getting out of equilibrium with the translational temperature, as can be seen from the figure. Through a shock wave, the temperature associated with the translational motion, T_{trans}, increase more rapidly than the temperature corresponding to the rotational motion (T_{rot}), while in strong expansions, the opposite effect can be observed.

The present work focuses on the recent development of molecular dynamics modelling of diatomic gas flows in strong thermodynamic non-equilibrium and the coupling of the molecular-level modelling to mesh-based kinetic models. In particular, the development

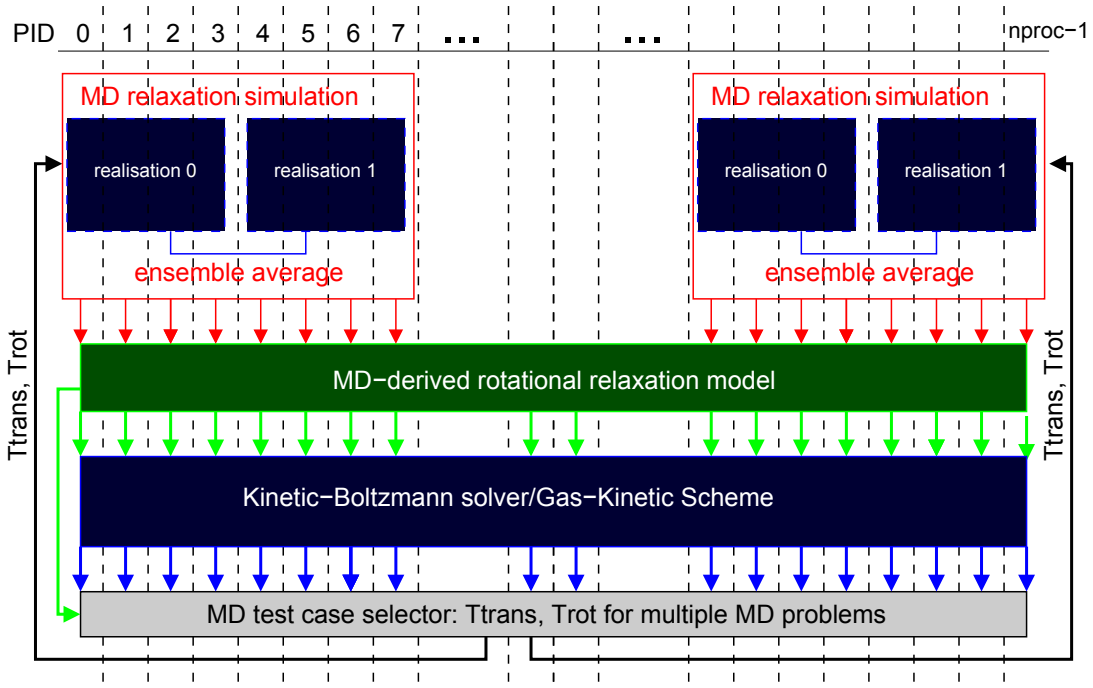


Figure 2: Multi-physics simulation of diatomic gas flow in thermodynamic non-equilibrium with a rotational-relaxation model based on multiple-sample MD simulations.

of a multi-physics simulation approach in which the rotational-relaxation model in the kinetic-Boltzmann solver takes detailed information from a series of molecular dynamics (MD) simulations. The rotational motion of diatomic molecules is assumed to be fully excited degrees of freedom, for which a classical MD model can be used, while, at present, it is assumed that the temperatures stay sufficiently low so that vibrational excitation present in high-temperature conditions plays a negligible role. Figure 2 sketches the principle of the multi-physics approach, where an 'MD-layer' is created in which all processes in a parallel simulation are involved in conducting multiple MD simulations representing a number of thermodynamic non-equilibrium situations. For each of these conditions, multiple realisations are created and ensemble-averaging is then used to feed the information into an empirical rotational-relaxation model, which is used in the flow simulation conducted using either of the following approaches: (i) a Gas Kinetic Scheme (GKS) based on the Rykov model recently developed by the authors[7] is used throughout the flow domain, (ii) a discrete-velocity method (DVM) for the Rykov or diatomic-ES model is used or (iii) a hybrid approach coupling the GKS and the DVM methods. In the following, the development of the multi-physics approach as well as results from MD modelling of rotational relaxation at conditions representative of hypersonic flows around aerospace vehicles are discussed along with the steps involved in the further development of the multi-physics approach in MΦC.

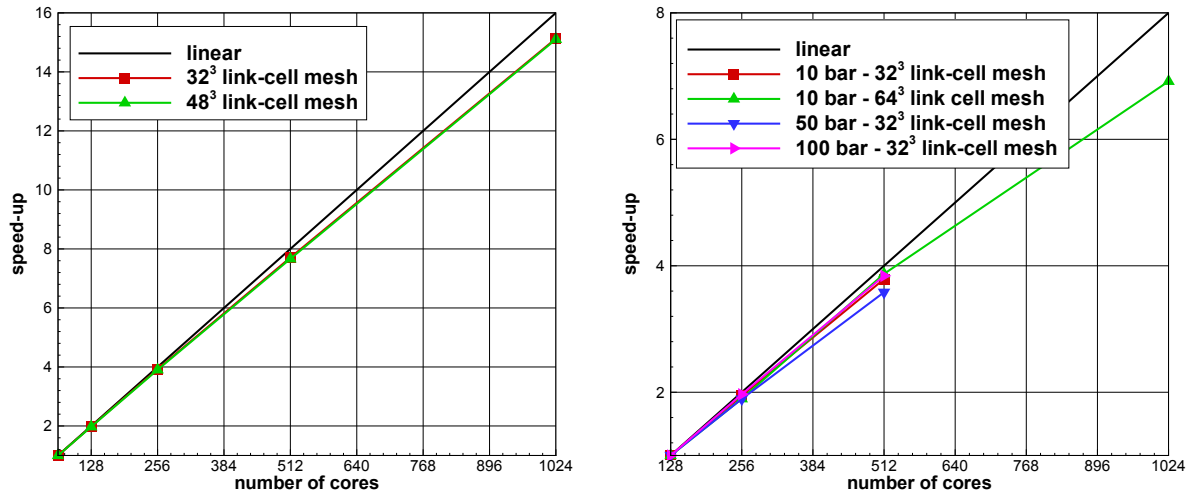


Figure 3: Multi-sample MD simulation. Parallel speed-up for liquid water (two different domain size) and for nitrogen gas at different pressures. Timings recorded on IBM BlueGene/Q machine.

2 MULTI-PHYSICS SIMULATION - MΦC FRAMEWORK

The framework was designed starting from a generalisation of the domain-decomposition paradigm, i.e. the particle-based and mesh-based methods included in the framework were designed for large-scale parallel simulation with sub-domains divided across multiple processes. For hybrid simulations coupling different models and methods, data is exchanged using message passing between the different domains. Generic container and iterator classes were created, along with classes to define problem topology, message-passing based data transfer, etc. A high level of abstraction was used in the basic classes such that re-use of software, i.e. the C++ template classes in the framework's library, can be used for both particle-based and mesh-based methods for a range of mathematical models.

3 MΦC - MOLECULAR DYNAMICS SOLVER

The MD solver employs a linked-cell list algorithm to determine the interaction for each molecule with its neighbours within a predefined interaction range. The rectangular domain is split in multiple sub-domains for parallel computation. For non-linear molecules, a quaternion formulation is used to define the rotational motion of the molecule[8]. A predictor-corrector method is used for the time integration. The main class defining a cell in the linked-cell method is defined as,

```
// class T = particle class
// class U = link-cell container iterator
// class V = data storage class
// class W = data storage class for translation
template <class T,class U,class V,class W>
```

```
class MD_Quat_Cell {
    ...
};
```

The particle class `T` in the template class `MD_Quat_Cell` for a non-linear molecule (e.g. water) is defined as,

```
class WaterQuat {
    int sitesMol; // Number of 'sites' within molecule
    VecR mol_r, mol_rv, mol_ra, mol_ra1, mol_ra2, mol_ro, mol_rvo;
    Quat mol_q, mol_qv, mol_qa, mol_qa1, mol_qa2, mol_qo, mol_qvo;
    VecR *site_force; // forces acting on molecule 'sites'
    ...
};
```

In the parallel data exchange, molecule positions and orientations need to be exchanged between process to correctly define the particles in the 'halo' cells. Furthermore, molecules will migrate from cell to cell in the linked-cell method, which might also involve the migration to another process. For the non-linear molecules, e.g. defined through class `WaterQuat`, the following structures are defined,

```
typedef struct {
    int icell;
    int ic,jc,kc;
    double pos[NDim+NQuat]; // mol_r , mol_q
    double vel[NDim+NQuat]; // mol_rv, mol_qv
} MD_ParticleQuatData;

typedef struct {
    int icell;
    int ic,jc,kc;
    double pos[NDim+NQuat]; // mol_r , mol_q
    double vel[NDim+NQuat]; // mol_rv, mol_qv
    double acc[3*NDim+3*NQuat]; // mol_ra, mol_ra1, mol_ra2, mol_qa, mol_qa1, mol_qa2
} MD_ParticleQuatTrans;
```

where `NQuat`=4 and `NDim`=3. These datatypes are used as templates `V` and `W` in class `MD_Quat_Cell`, respectively.

For linear molecules, with only two rotational degrees of freedom rather than three, a simplified model[8] is used in the MD solver. In this model, the torque on a molecule is defined as,

$$\vec{n} \;=\; \sum_k \vec{r} \times \vec{f_k} = \vec{s} \times \sum_k d_k \vec{f_k} = \vec{s} \times \vec{g} \tag{1}$$

where the orientation is defined by $\vec{s}$, the unit vector along the molecular axis, and where d_k is the signed distance along the axis of each interaction site from the centre of mass. For the linear nitrogen molecule considered in the present work, the angular momentum is $I\vec{\omega}$, with I the moment of inertia about the two principal axes, giving the following equations for the rotational motion,

$$I\frac{d\vec{\omega}}{dt} = \vec{s}\times\vec{g} \quad ; \quad \frac{d\vec{s}}{dt} = \vec{\omega}\times\vec{s} \tag{2}$$

$$I\frac{d^2\vec{s}}{dt^2} = \vec{g} - \left[\left(\vec{s}\cdot\vec{g}\right) + I\frac{d\vec{s}}{dt}\cdot\frac{d\vec{s}}{dt}\right]\vec{s} \tag{3}$$

Equation (3) along with the equations of motion for the translational motion are integrated using a predictor-corrector method. For the linear-molecule case, modified versions of the above C++ classes are used, while the main container, iterator and message-passing classes are identical.

3.1 Liquid water and nitrogen gas models

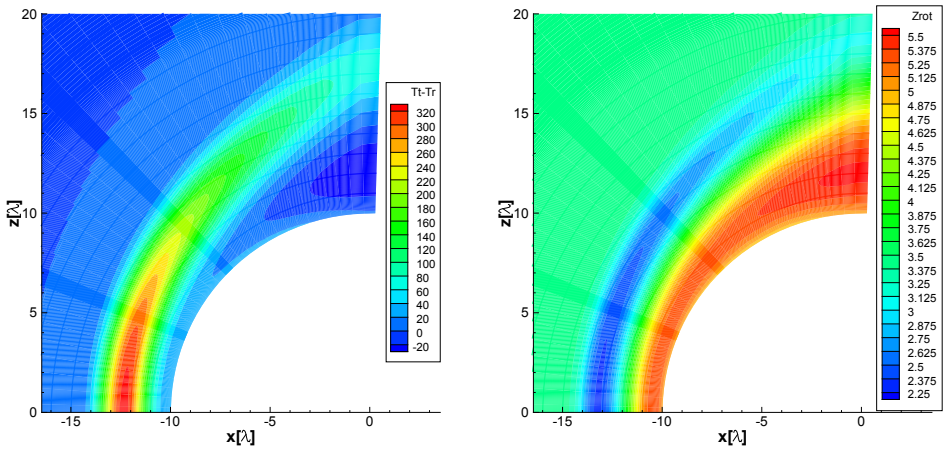
The MD solver in MΦC was first validated using a number of test cases for liquid water. For MD simulations of liquid water, the well-known TIP4P water model was used. The model molecule is based on four interaction sites located in a planar configuration. For the Lennard-Jones (LJ) part of the potential, the potential well depth is taken as $\epsilon/k_B = 78.2$. In the simulations, the problem is non-dimensionalised in LJ units. The interaction cutoff is $r_c = 7.5$ Å or 2.38σ.

For MD simulations of nitrogen gas, a Lennard-Jones based model was used with two sites on each molecule coinciding with the atom locations. The potential well depth is taken as $\epsilon/k_B = 37.3$, while a reduced length $\sigma = 3.31$ Å was used. For the linear molecule, the moment of inertia about the two axes with non-zero inertia is defined by a radius of gyration of 0.0547 Å.

3.2 Parallel performance

The parallel speed-up was investigated for a number of different multi-sample MD simulations on the BlueGene/Q computer at the Hartree Centre in the UK. Figure 3 presents the parallel speed-up for the liquid water as well as the nitrogen gas test cases. For liquid water, a temperature of $298K$ and density of $1000kg/m^3$ were used. In LJ units, the employed time step was 0.0005. The cases with 32^3 and 48^3 cells in the cell-linked list correspond to 2.10 and 6.97 million molecules, respectively. The simulations used 4 realisations, with the number of cores per realisation increasing from 16 to 256, with a parallel efficiency of 94%. For the nitrogen cases, the 10, 50 and 100 bar cases correspond to 32768, 110592 and 262144 molecules for the cases with 32^3 cells in the cell-linked list. For 10 bar, a case with 64^3 cells was also considered. In LJ units, the employed time step was 0.000025. The nitrogen simulations used 64 realisations, so that the number of cores per realisation varied from 2 to 16 and a parallel efficiency of approximately 80% was observed. For the water simulations, the number of molecules each of the molecules interacts with is significantly higher than in any of the nitrogen gas cases. Therefore, within each of the cells of the cell-linked list formulation used, the liquid water simulations have a significantly larger number of molecules than the cells in the nitrogen gas

simulations. Furthermore, the molecules in the liquid phase are far more uniformly distributed in space as compared with especially the low-density gas simulations. For these reasons, the present parallel simulations based on the spatial domain-decomposition approach show a better parallel speed-up for the water simulations than for the nitrogen simulations. However, the obtained results indicate that for a suitable chosen set of samples, a good parallel speed-up can be achieved for MD simulations of nitrogen gas with multiple realisations.



(a) $T_{trans} - T_{rot}$ (b) $Z_r(T_{trans}, T_{rot})$

Figure 4: Rarefied Mach 5 flow over sphere simulated using the Rykov-based Gas Kinetic Scheme. Free-stream temperature $T_\infty = 116K$, wall temperature $290K$. sphere radius 10 mean-free path lengths at free-stream conditions (λ).

4 MΦC - GRID-BASED KINETIC-BOLTZMANN SOLVERS

Using the container and iterator classes in MΦC, cell-centred finite-volume methods were created for the simulation of kinetic-Boltzmann models using a Gas Kinetic Scheme (GKS) based on the Rykov model recently developed by the authors[7]. A discrete-velocity method (DVM) for the kinetic models as well as hybrid approaches coupling the GKS and the DVM methods have also been developed. In the present work, the focus is on diatomic gas flows modelled with the Rykov model, which is a kinetic-Boltzmann model in which the rotational degree of freedom of the molecules is taken into account using an additional particle distribution function compared to a monoatomic kinetic model. The two particle distribution functions in the Rykov model are governed by the following equations,

$$\frac{\partial F_0}{\partial t} + \mathbf{c}\frac{\partial F_0}{\partial \mathbf{x}} = \frac{F_0^{eq} - F_0}{\tau} \quad ; \quad \frac{\partial F_1}{\partial t} + \mathbf{c}\frac{\partial F_1}{\partial \mathbf{x}} = \frac{F_1^{eq} - F_1}{\tau} \tag{4}$$
$$F_0^{eq} = \frac{1}{Z_r}F_0^r + \left(1 - \frac{1}{Z_r}\right)F_0^t \quad ; \quad F_1^{eq} = \frac{1}{Z_r}F_1^r + \left(1 - \frac{1}{Z_r}\right)F_1^t$$

with F_0^r, F_0^t, F_1^r, F_1^t modified equilibrium functions involving translational as well as rotational temperature. The total collision time τ is expressed as μ_t/p with the viscosity and pressure determined from the translational temperature. The Rykov model is based on the assumption that the fraction of collisions involving the excitation of the rotational degrees of freedom, Z_r, is a given constant or a function of the flow temperatures. In the present work, Z_r will be investigated in more detail using molecular dynamics in section 5.

Gas Kinetic Schemes (GKS) are a class of methods in which the numerical flux across through cell faces in a finite-volume method is derived from a local kinetic problem around the cell interfaces. In the present work, this flux includes both convective and and viscous contributions but is more expensive than Roe or AUSM fluxes with central discretisation of the viscous fluxes. The Rykov-based GKS was defined starting from Equation (4). The non-equilibrium particle distribution functions were defined using a Chapman-Enskog expansion, which limits the scheme to moderate levels of thermal non-equilibrium. Integrating in time for a one-dimensional flow in a control volume dx with a continuous particle velocity c_x and discretised space x_i and time t^n, with step sizes of Δx and Δt respectively, one obtains

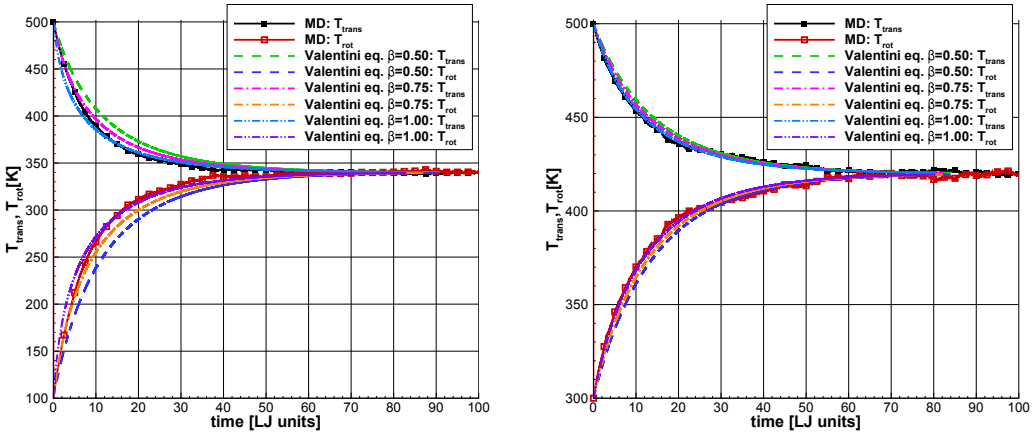
$$F|_i^{n+1} = F|_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} \left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) dt + \frac{\Delta t}{2}\left(\frac{F|_i^{n+1} - F|_i^{n+1}}{\tau^{n+1}} + \frac{F|_i^n - F|_i^n}{\tau^n}\right)$$

where the trapezoidal rule has been employed for the collision term integral, S, and $[c_x F]|_{i\mp 1/2}$ are the fluxes of the distribution function across the cell interface. Then, taking the moments $\hat{\mathbf{\Psi}} = (1,\ c_x,\ \mathbf{c}^2)^T$ of equation above, the update of the conservative variables can be found as

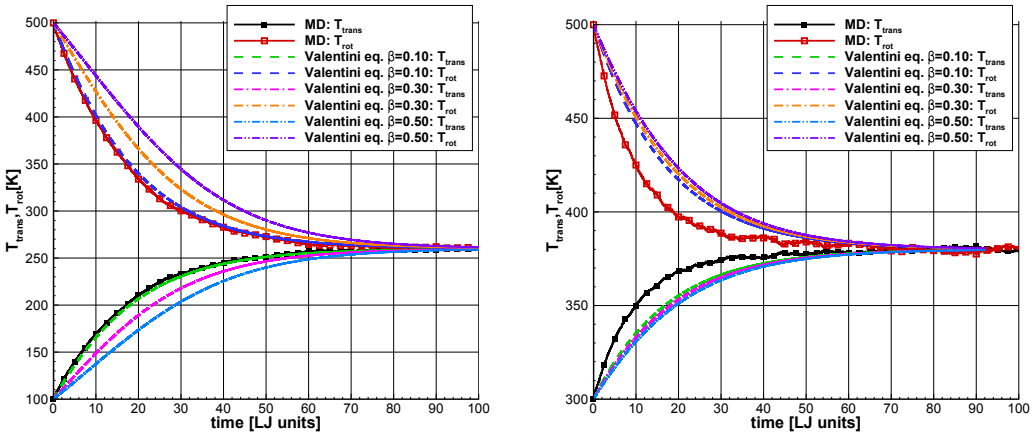
$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}\left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) d\mathbf{c}dt + \frac{\Delta t}{2}\left(S^{n+1} + S^n\right) \quad (5)$$

5 MD MODELLING OF ROTATIONAL RELAXATION IN NITROGEN

In a system of colliding particles, energy is transferred between the various internal modes. These collisions tend to drive the internal energy distributions towards their respective equilibrium state. In a diatomic gas, the time required for the different modes to relax towards the equilibrium state is different, i.e. the translational motion generally approaches its equilibrium faster than the rotational motion of the gas. For the rotational relaxation time we can then write $\tau_r = Z_r\tau$, where τ is the translational relaxation time and $Z_r > 1$ the rotational collision number. Theoretical works by Parker[9] and Lordi and Mates[10] considered pairs of molecules sampled from equilibrium conditions for the considered temperature to create empirical expressions for the rotational collision



Initial $T_{trans} > T_{rot}$



Initial $T_{rot} > T_{trans}$

Figure 5: MD simulation of rotational relaxation in nitrogen. Non-equilibrium initial conditions with translational temperature exceeding the rotational temperature is representative of strong gas compression through shock wave. Non-equilibrium initial conditions with rotational temperature exceeding the translational temperature are representative of strong expansions.

number as function of temperature. Despite the fact that Parker's work involved a large number of simplifying assumptions such as a restriction to co-planar collisions to enable an analytical treatment, the overall dependence on the temperature is in agreement with the more rigorous numerical analysis of Lordi and Mates[10], who also considered general non-planar collisions. In the literature, empirical formulas derived from data fitting, either from numerical or experimental results, have been presented. Valentini and co-workers derived an expression for $Z_r(T_{trans}, T_{rot})$ derived from molecular dynamics simulations,

defined as,

$$Z_r = \left[a_1 \left(\frac{T_{trans}}{1K}\right)^{1/4} + a_2 \left(\frac{T_{trans}}{1K}\right)^{-1/4} - a_3 \left(\frac{T_{trans}}{1K} - 1000\right)\right] \left[1 - \beta \left(1 - \frac{T_{rot}}{T_{trans}}\right)\right] \quad (6)$$

where $a_1 = 1.33868$, $a_2 = -6.19992$, $a_3 = -0.00107942$ and $0 < \beta \leq 1$. In their work, Valentini et al. performed a series of adiabatic and isothermal MD simulation starting from a non-equilibrium gas state, in which the translational and rotational motions were sampled from Maxwellians at different temperatures. The emphasis was on the situation in which the translational temperature exceeds the rotational temperature, i.e. representative of the situation downstream of a strong shock wave in a high-Mach number flow.

Figure 4 presents results for the Mach 5 flow around a sphere obtained with the Rykov GKS method. The shock can be seen to create a difference in translational and rotational temperatures of the order of $300K$ with the considered free-stream temperature of $116K$, while the expansion over the sphere leads to smaller differences. Figure 4(b) shows Z_r evaluated using Equation (6) with $\beta = 1$ as used in the simulation.

For the proposed multi-physics approach, the Z_r, which for Rykov GKS simulations appears in the equilibrium functions as well as the relaxation source term S, is to be evaluated using an equation of the type (6) which is then adjusted and extended with MD-derived data. As a first step, the rotational relaxation for non-equilibrium conditions observed in Figure 4(a) are analysed using the MD solver in MΦC.

A cubic domain with dimensions $[154.9\sigma_{LJ}]^3$ was created with 32768 molecules. For the gas at $298K$ this would correspond to a pressure of 10 bar. For all simulations, the molecules were initialized on a regular lattice with random velocity vectors sampled from a Maxwellian distribution. First, an equilibration phase was conducted during $10\tau_{LJ}$ reduced time units. Then, an non-equilibrium situation was created by rescaling either the rotational motions or translational motions, to adjust the rotational or translational temperature, respectively. During this non-equilibrium phase of the simulation, no thermostat was applied and a sufficiently small time-step was used to prevent excessive numerical errors. A time step of $0.000025\tau_{LJ}$ was used in the simulations presented here.

The results from the MD simulations of nitrogen in rotational relaxation were analysed in detail by comparing the present results with those obtained using Valentini's expression, i.e. Equation (6). To compare the empirical expression for Z_r with the present MD results, the rotational relaxation in a gas at constant volume and total energy was simulated using the Jeans-Teller model for the relaxation term, a power-law model for the gas viscosity (based on the translational temperature T_t and $\omega = 0.74$) and expression for rotational relaxation time $Z_r\mu/p$, with the gas pressure evaluated from the constant density and the translational temperature. This problem was integrated in time using a 4th-order accurate Runge-Kutta method until the two temperatures were within a small predefined tolerance. In the following, the values for the constant a_1, a_2, a_3 were those reported[11], while the constant $0 < \beta \leq 1$. For the non-equilibrium MD simulations with $T_{trans} > T_{rot}$

a very good agreement with Valentini's fit was found for β was close to 1, as can be see from Figure 5. For the opposite situation, i.e. $T_{rot} > T_{trans}$ (which was not considered by Valentini et al.), using Equation (6) with β similarly close to 1 was found to give a poor agreement. By reducing β to approximately 0.1 a better agreement with the present MD results can be seen for some of the cases considered, as shown in the plots in the bottom row of Figure 5. For some of the considered conditions, the empirical expression needs an adjustment to the constants a_1, a_2, a_3 to create a match.

For the multi-physics approach defined in Figure 2, the relaxation-model gets refined and adjusted during the course of the flow simulation. The MD test case selection step should involve criteria defining the validity of the used relaxation-model in terms of which thermodynamic non-equilibrium condition which can be reliably modelled with the relaxation model and for which conditions further MD simulations need to be initiated.

6 CONCLUSIONS

The development of a multi-physics solution method for hypersonic rarefied flows was described. For the implementation in the MΦC framework, the re-use of C++ template classes available in the template-class library to unify the source for the particle-based and mesh-based solvers were described. The simulation of rotational relaxation in nitrogen gas, the Molecular Dynamics solver was analysed in detail and the obtained results were compared against available data in the literature. For gas conditions representative of strong expansion regions, it was found that available empirical models may be inadequate and that therefore the proposed multi-physics approach in which the MD simulations are integrated with the flow simulation may provide an important step forward, provided sufficient computer resources are available. Future work will analyse how best to integrate the MD-derived data into a rotational-relaxation model in the context of hybrid simulations based on kinetic Boltzmann models.

ACKNOWLEDGEMENT

The financial support by the University of Liverpool is gratefully acknowledged. We acknowledge PRACE for awarding us access to SuperMUC based in Germany at the Leibniz Rechenzentrum (LRZ) in Munich. Furthermore, we would like to acknowledge the Hartree Centre in the UK for access to the BlueGene/Q through the BlueJoule Access Programme.

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